

4/24

OPTIONAL FORM 69 (7-90)

**FAX TRANSMITTAL**

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NSN 7540-01-317-7868

5099-101

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GENERAL SERVICES ADMINISTRATION

Jon,

The following depictions are from the EPA/NIH Mass spectral database, which should show you the structural differences between the isomers.

I've also attached a page from the Merck index which says that "Bis(2-ethyl hexyl)phthalate" and "Diethyl phthalate" describe the same compound but we know that the bis(2ethylhexyl)ester and the diethyl ester are structural isomers.

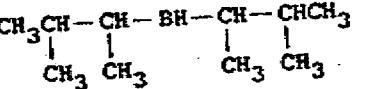
If I were you, I'd try to go by the EPA/NIH list. Call if you have further questions.

Lisa Gattan

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selective reductions. G. W. Bratt. *J. Am. Chem. Soc.* 98, 167 (1976).

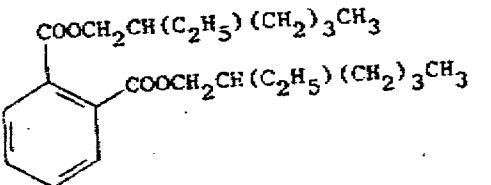
Tech. 6, 324 (1976).



Crystals, mp 35-40°. Unstable to air.

USE: Selective reagent for steric control of hydroboration of olefins.

1248. Bis(2-ethylhexyl) Phthalate. *1,2-Benzenedicarboxylic acid bis(2-ethylhexyl) ester; di(2-ethylhexyl) phthalate; diethyl phthalate; Octoil.*  $\text{C}_{14}\text{H}_{38}\text{O}_4$ ; mol wt 390.54. C 73.80%, H 9.81%, O 16.39%. Prepn: Garner, Watson, U.S. pat. 2,508,911 (1950 to Shell); Brit. pat. 747,260 (1956 to Chemische Werke Hüls).



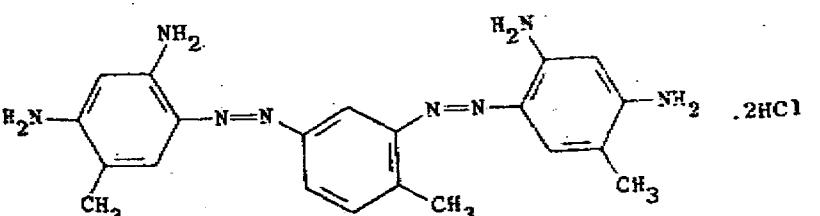
USE: In vacuum pumps.

1249. Bis(2-ethylhexyl) Sebacate. *Decanedioic acid bis(2-ethylhexyl) ester; di(2-ethylhexyl) sebacate; Octoil S; Plexol 201.*  $\text{C}_{16}\text{H}_{38}\text{O}_4$ ; mol wt 426.66. C 73.19%, H 11.81%, O 15.00%.  $\text{CH}_3(\text{CH}_2)_3\text{CH}(\text{C}_2\text{H}_5)\text{CH}_2\text{OOC}(\text{CH}_2)_8\text{COOCH}_2\text{CH}(\text{C}_2\text{H}_5)(\text{CH}_2)_3\text{CH}_3$ . Prepn: Bruno, U.S. pat. 2,628,249 (1953 to Pittsburgh Coke & Chemical); Brit. pat. 747,260 (1956 to Chemische Werke Hüls).

Liquid,  $d_{40}^{25}$  0.9119,  $n_D^{25}$  1.4496.

USE: In vacuum pumps.

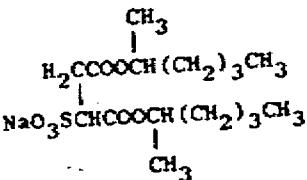
1250. Bismark Brown R. *4,4'-[4-Methyl-1,3-phenylene]bis(azo)]bis[6-methyl-1,3-benzenediamine] dihydrochloride; C.I. Basic Brown 4; 5,5'-[(4-methyl-m-phenylene)bis(azo)]bis[toluene-2,4-diamine] dihydrochloride; C.I. 21010; Bismark Brown 53; Vesuvine.*  $\text{C}_{21}\text{H}_{26}\text{Cl}_2\text{N}_4$ ; mol wt 461.41. C 54.67%, H 5.68%, Cl 15.37%, N 24.29%. Prepd by reaction of toluene-2,4-diamine HCl with nitrous acid: Colour Index vol. 4 (3rd ed., 1971) p 4154.



Blackish-brown powder. Very sol in water; slightly sol in ethanol, Cellosolve; practically insol in acetone, benzene carbon tetrachloride. In concd  $\text{H}_2\text{SO}_4$  gives brown soln; in concd nitric acid gives orange soln which turns yellow.

USE: As a textile dye, biological stain.

1252. Bis(1-methylamyl) Sodium Sulfosuccinate. *Sulfobutanedioic acid 1,4-bis(1-methylpentyl) ester sodium salt; dimethyl sodium sulfosuccinate; Aerosol MA; Alphasol MA.*  $\text{C}_{16}\text{H}_{29}\text{NaO}_7\text{S}$ ; mol wt 388.46. C 49.47%, H 7.53%, Na 5.32%, O 28.83%, S 8.25%. The bis(1-methylamyl) ester of sulfosuccinic acid monosodium salt, perhaps in admixture with the dihexyl ester. Prepd by the action of the appropriate alcohols on maleic anhydride followed by addition of sodium bisulfite: Jaeger, U.S. pats. 2,028,091; 2,176,423; Brit. pat. 446,568; Fr. pat. 776,495 (to Am. Cyanamid).



Available as white, slightly hygroscopic, wax-like pellets. Must be soaked to dissolve in cold water. Dissolves rapidly in hot water. Solubility in water at 25° = 343 g/l; at 70° = 447 g/l. Maximum concn of electrolyte soln in which 1% of the wetting agent is sol: 2% NaCl; 2%  $\text{NH}_4\text{Cl}$ ; 14%  $(\text{NH}_4)_2\text{HPO}_4$ ; 3%  $\text{NaNO}_3$  (slightly turbid); 3%  $\text{Na}_2\text{SO}_4$ . Also sol in pine oil, oleic acid, acetone, kerosene, carbon tetrachloride, 2B ethanol, benzene, hot olive oil, glycerol. Insol in liquid petrolatum. Stable in acid and neutral solns, hydrolyzes in alkaline solns.

USE: Wetting agent.

1253. Bis[methylthio]methane. *Bis[methylmercapto]methane; methylenebis[methyl sulfide].*  $\text{C}_3\text{H}_8\text{S}_2$ ; mol wt 108.21. C 33.30%, H 7.45%, S 59.25%.  $(\text{CH}_3\text{S})_2\text{CH}_2$ . Odorous principle of the white truffle *Tuber magnatum* (Pico) Vitt., Tuberaceae. Isoln: Fiechti et al., *Tetrahedron Letters* 1967, 1681. Synthesis from methyl mercaptan: Böhme, Marx, *Ber.* 74, 1672 (1941).

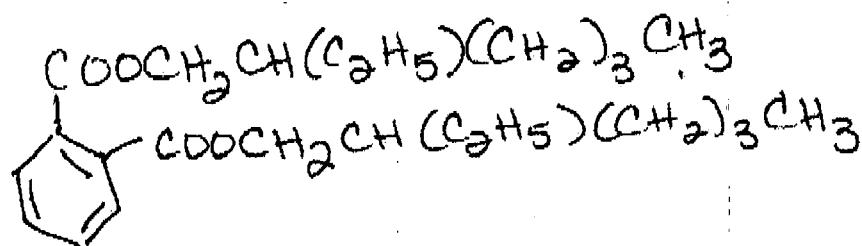
Oily liquid. Odor in high dilutions reminiscent of white truffles. The odor of the neat liquid resembles that of freshly prep'd mustard without its acrid and irritating qualities. bp 148-149°. Mass spectra: Fiechti, loc. cit.

1254. Bismuth. Bi; at. wt 208.9804; at. no. 83; valence 3. One naturally occurring isotope: 209; artificial radioactive isotopes: 199-208; 210-215. Confused with tin until 1450. First isolated by Hillot in 1737. It was, however, Geoffrey the Younger who clearly proved its individuality in 1750. Bismut and Bergmann are named as the scientific dis-

$C_{24}H_{38}O_4$ 

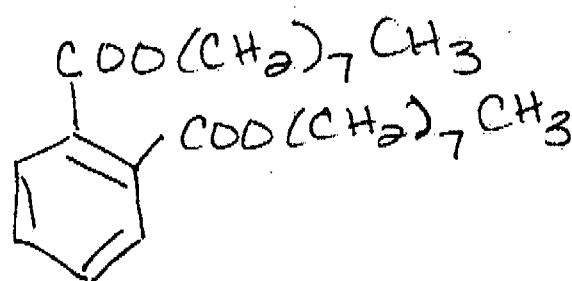
Cas. # 117-81-7

1,2-Benzenedicarboxylic acid, bis( $\omega$ -ethyl hexyl)ester

 $C_{24}H_{38}O_4$ 

Cas. # 117-84-0

1,2-Benzenedicarboxylic acid, dioctyl ester

 $C_{24}H_{38}O_4$ 

Cas. # 27554-26-3

1,2-Benzenedicarboxylic acid, diisooctyl ester

